

2-Chloroethanol
107-07-3 | DTXSID1021877

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.97 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.78e-01

Confidence level: 5.76e-01

Nearest Neighbors from the Training Set

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2-Chloroethanol

Measured: 12.4

Predicted: 4.97

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3-Chloro-1-propanol

Measured: 2.64

Predicted: 2.43

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2,2,2-Trichloroethanol

Measured: 5.58e-01

Predicted: 5.36e-01

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3-Chloro-2-butanol

Measured: 6.13e-01

Predicted: 6.25e-01

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3-Pyridinol

Measured: 3.50e-01

Predicted: 9.48